Peter Graf

Current Affiliation: National Renewable Energy Laboratory, Materials and Computational Sciences Center, Scientific Computing Group
Role in Center: High-performance computer simulation and optimization

Education and Training

- Stanford University, Symbolic Systems / Artificial intelligence, B.S., 1989
- University of California at Berkeley, Mathematics / Model reduction for ordinary differential equations, Ph.D., 2003
- NREL, Scientific Computing Center / Simulation Optimization, Postdoctoral training: 2003–2006

Research and Professional Experience

- Scientist II, NREL, Scientific Computing Group. High performance computing. Applied mathematics. Modeling, simulation, optimization, data mining in support of a variety of renewable energy research. Mathematical research in simulation optimization, 2006–present
- Postdoctoral Research Associate, NREL, Scientific Computing Center. Simulation optimization for alloys and nanostructures, 2003–2006
- Graduate Research Associate, Lawrence Berkeley National Laboratory. Mathematical research in optimal prediction and other model reduction techniques for differential equations, 1998–2002
- C/C++ Programmer, Access Softek, Inc. Berkeley, Ca. Windows and Macintosh commercial programmer. Highlights from a wide variety of projects include genetic programming based optimization for physical simulation of articulated figures, 1992–1997

Relevant Publications

- M. Kose, P. Graf, N. Kopidakis, S. Shaheen, K. Kim, and G. Rumbles, 2008, Exciton Migration in Conjugated Dendrimers: A Joint Experimental and Theoretical Study, *J. Am. Chem. Soc.* (submitted).
- P. A. Graf, W. B. Jones, 2008, A Scatter Search Based Inverse Band Structure Method for Semiconductor Alloys, *J. Comput. Phys.* (submitted).
- P. Piquini, P. A. Graf, and A. Zunger, 2008, Band-gap Design of Quaternary (In,Ga)(As,Sb) Semiconductors Via the Inverse-band-structure Approach, *Phys. Rev. Lett.* **100**, 2008; pp. 186403.
- P. A. Graf and W. B Jones, Optimization of Semiconductor Alloy Properties Using the Virtual Crystal Approximation, *J. Comput. Phys.* (accepted, 2008).
- P. A. Graf and W. B. Jones (2007). A Projection Based Multiscale Optimization Method for Eigenvalue Problems. *J. Global Optim.* **39**, 2007; pp. 235-245.
- P. A. Graf, K. Kim, W. B. Jones, and L.-W. Wang, (2007). Surface Passivation Optimization Using DIRECT. *J. Comput. Phys.* **224**(2), 2007; pp. 824-835.
- Q. Zhao, P.A. Graf, W.B. Jones, A. Franceschetti, J. Li, L. Wang, and K. Kim, (2007). Shape Dependence of Band-Edge Exciton Fine Structure in CdSe Nanocrystals. *Nano Letters.* **7**(11), 2007; pp. 3274-3280.
- G. Trimarchi, P. Graf, and A. Zunger (2006). Exploring the Configurational Space of Binary Alloys: Different Sampling for Different Cell Shapes. *Physical Review. B, Condensed Matter and Materials Physics* **74**(1), 2006, 32.

- K. Kim, P.A. Graf, and W.B. Jones (2005). A Genetic Algorithm Based Inverse Band Structure Method for Semiconductor Alloys. *Journal of Computational Physics* **208**(2), 2005; pp. 735-760.
- P.A. Graf, K. Kim, W.B Jones, and G.L.W. Hart (2005). Direct Enumeration of Alloy Configurations for Electronic Structural Properties. Applied Physics Letters **87**(24), 2005; 3 pp.

Synergistic Activities

- Member of SciDAC II project: Green Energy: Advancing Bio-hydrogen. Developing a model of metabolism linked to H2 production in green algae.
- Member of SciDAC I project: Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures.
- NREL LDRD proposal submitted: Simulation strategies for organic, excitonic and third-generation solar cells.
- Member of 2008 SuperComputing (SC08) conference applications papers program committee.
- Participated it Computational Research Needs in Alternative and Renewable Energy (CRNARE) workshop, Sept. 07.